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Topology-Induced Inverse Phase Transitions

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Abstract – Inverse phase transitions are striking phenomena in which an apparently more ordered state disorders under cooling. This behavior can naturally emerge in tricritical systems on heterogeneous networks and it is strongly enhanced by the presence of disassortative degree correlations. We show it both analytically and numerically, providing also a microscopic interpretation of inverse transitions in terms of freezing of sparse subgraphs and coupling renormalization.

Introduction. – Network-based representations are appropriate tools to describe many real-world systems and to classify their structural and functional properties using few topological measures, such as for instance the degree distribution, degree correlations and clustering [1]. Networks characterized by degree distributions with power-law tails have attracted a lot of attention, mostly because of their unusual structural and dynamical properties [2–4]. However these studies are mostly limited to uncorrelated random graphs, i.e. graphs characterized solely by their degree distribution. Many real-world networks show instead degree correlations. For instance, social networks are usually characterized by positive degree correlations (assortative mixing), because high-degree nodes tend to be directly connected and to form cliques [5]. In technological and biological networks, instead, the hubs are preferentially connected to low degree nodes (disassortative mixing) [6]. Degree correlations can strongly affect the overall behavior of dynamical processes, as it was recently shown for percolation [7] and diffusion processes [8].

In this Letter, we show that some amount of degree heterogeneity and negative degree correlations can be responsible for the occurrence of inverse phase transitions. The latter are counterintuitive phenomena in which a system, starting from a high temperature disordered phase first undergoes a phase transition to a more ordered phase than comes back to a disordered one as a result of monotonic decrease of temperature. Examples of this curious behavior

are observed in a variety of systems, such as liquid binary mixtures, ^{3}He-^{4}He isotopes, ultra-thin films, liquid crystals, disordered high-T superconductors and polymeric solutions [9]. An inverse transition implies the inversion of the standard ratio between the entropic content of the two phases [10]. This behavior has a simple microscopic explanation for some systems, such as water solutions of methyl-cellulose polymers, in which the more interacting unfolded state is entropically favored because it admits many more microscopic configurations than the non-interacting folded one. As suggested by the Flory- Huggins theory of polymer melts [11], a general way of triggering an inverse phase transition is to introduce a temperature-dependent interaction. This latter naturally emerges in spin systems with higher degeneracy of interacting states [12]. Moreover, an inverse freezing transition between glassy and paramagnetic phases exists in tricritical spin glasses [13], [14], [15] and in spin-glasses on small world graphs [16].

Here we study the tricritical Ising model defined on random graphs, providing evidence of a novel topological mechanism that is responsible of an inverse melting transition. Using the cavity method, we show that degree fluctuations can generate a reentrance in the low temperature region of the phase diagram. The physical reason at the origin of this behavior is identified in the partial freezing of the microscopic degrees of freedom that generates a temperature-dependent renormalization of the effective interaction couplings. The mechanism, that requires some amount of degree heterogeneity to occur, is amplified by
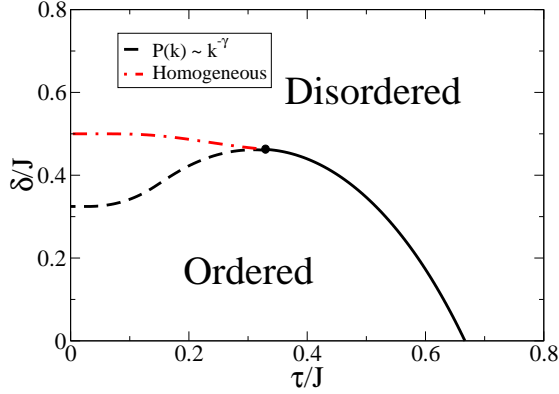
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Fig. 1: Phase diagram (τ, δ) of the Blume-Capel model in the Curie-Weiss approximation for random graphs. The second order continuous branch has the universal scaling form of the Eq.3. The first order discontinuous branches are different for homogeneous (random regular graph of degree $K = 5$) and heterogeneous graphs (random graph with power-law degree distribution $P(k) \propto k^{-\gamma}$, with $\gamma = 3.5$) respectively.

disassortative mixing. This is of great relevance because many real-world technological and biological networks are disassortative and degree anti-correlations have been recently shown to be a natural feature of heterogeneous networks [17].

The Model. – The tricritical Ising model, known as Blume-Capel (BC) model [18], describes spin-1 variables $s_i = \{0, \pm 1\}$ defined on the sites of a lattice or a graph, and interacting according to the Hamiltonian

$$H_{BC} = -J \sum_{\langle i,j \rangle} s_i s_j + \Delta \sum_i s_i^2 \qquad (1)$$

where the first sum runs over nearest neighbor pairs $\langle i, j \rangle$ and the chemical potential Δ controls the density. It is well known that the BC model exhibits a rich $T - \Delta$ phase diagram with lines of first-order and second-order phase transitions dividing the ferromagnetic phase at low temperature T and chemical potential Δ from the paramagnetic phase at large T and/or Δ [18]. The composition of the paramagnetic phase changes gradually and continuously from a purely disordered one (spins ± 1) at large T and low Δ, to a vacancy-dominated state for large Δ and low T. In the following, we consider spins defined on the nodes of an uncorrelated random graph with degree sequence $k_1, k_2, \ldots, k_N$ randomly drawn from a given degree probability distribution $P(k)$.

Role of Degree Heterogeneity. – A qualitative insight on the role played by degree heterogeneity in determining the critical behavior of the BC model can be obtained within a Curie-Weiss (CW) approximation. This is comparable to an "annealed" or a "random neighbor" ap-

proximation where the adjacency matrix $a_{i,j}$[1] is replaced in the Hamiltonian by the probability $k_i k_j / \langle k \rangle N$ that the link between nodes i and j is present [2]. This approximation allows the factorization of the free energy and the analytic computation of the partition function by Gaussian integration. It follows that the magnetization μ of a neighbor of a randomly chosen site satisfies the mean-field self-consistent equation $\mu = F(\mu)$ where

$$F(\mu) = \sum_{k=k_{min}}^{k_{max}} \frac{kP(k)}{\langle k \rangle} \frac{\sinh(\beta k \mu)}{e^{\beta \Delta}/2 + \cosh(\beta k \mu)}. \qquad (2)$$

This equation has a paramagnetic solution $\mu = 0$ whose stability is determined imposing $F'(0) \leq 1$. Following Landau theory, the equation $F'(0) = 1$ defines a curve of second-order critical points between the paramagnetic and the ferromagnetic phases (the λ-line) till, upon decreasing the temperature, the third-order term in the free energy[2] expansion vanishes $F'''(0) = 0$ (the tricritical point), then the transition becomes first order and the aforementioned condition gives us only the location of the spinodal point beyond which the paramagnetic solution is not stable. In terms of the rescaled variables $\delta = \Delta \langle k \rangle / \langle k^2 \rangle$ and $\tau = T \langle k \rangle / \langle k^2 \rangle$ the λ-line has the form

$$\delta = \tau \log[2(1/\tau - 1)], \qquad (3)$$

whereas the tricritical point is $\tau_c = \frac{1}{3}$, $\delta_c = \frac{\log 4}{3}$, that coincides with the maximum of the curve Eq.3. Interestingly, the obtained mean-field λ-line depends on the graph properties only through the ratio $\langle k^2 \rangle / \langle k \rangle$, which determines the scaling factor.

Lowering the temperature beyond the tricritical point (τ_c, δ_c), we find a different dependence of the (first-order) transition line on the topological properties. It is useful to look directly to the $T = 0$ limit, where Eq. 2 becomes

$$\mu = \langle k\Theta(k\mu - \Delta)\rangle / \langle k \rangle \qquad (4)$$

and $\Theta(x)$ is the Heaviside step function. A direct calculation, done approximating sums on k with integrals, reveals the following behavior. For graphs with a degree distribution which falls off faster than k^{-3} for large k, we find that the ferromagnetic state with $\mu = 1$ is possible at $T = 0$ when $\Delta < k_{min}$. In order to access the stability property of this solution one needs to compare its energy $E[\mu] = -\langle k \rangle \mu^2 / 2 + \Delta \mu$ with the paramagnetic energy ($E = 0$) of the state with $s_i = 0$ $\forall i$. This shows that the $\mu = 1$ state is stable as long as $\Delta < \langle k \rangle / 2$. So for graphs with $k_{min} > \langle k \rangle / 2$, as for example graphs with $P(k) \simeq k^{-\gamma}$ and $\gamma > 3$, the coexistence region at $T = 0$ extends from $0 \leq \Delta \leq k_{min}$ with a first order phase transition at $\langle k \rangle / 2$. For scale free graphs with $2 \leq \gamma \leq 3$ the same arguments show that, at $T = 0$, a ferromagnetic state with $\mu \sim \Delta^{-\frac{3-\gamma}{\gamma-2}}$ exists for $\Delta < k_{max}$ and it is

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[1] $a_{i,j}$ is 1 if i and j are neighbors, 0 otherwise.
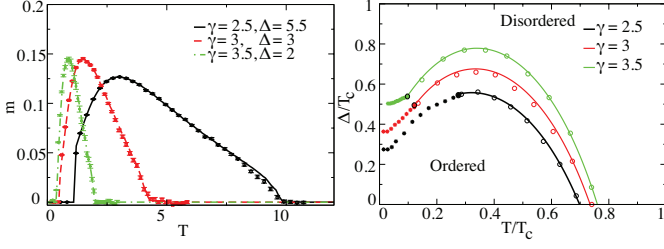[2] This can be obtained by integrating eq.2.

Fig. 2: Reentrant behavior in a random graph of size $N = 10^4$ and power-law degree distribution $P(k) \propto k^{-\gamma}$. Left) Curves $m(T)$ for different values of γ and Δ. Right) Phase diagram for $\gamma = 2.5, 3, 3.5$ obtained from the numerical solutions of the BP equations on single instances (points) and at the ensemble level (lines).

thermodynamically stable for $\Delta < (\langle k \rangle/2)^{\gamma-2}$. The same holds for $\gamma < 2$ with the important difference that $\langle k \rangle$ now diverges with k_{max} and that the magnetization μ is only weakly dependent on Δ.

Some of the results are summarized in Fig.1 which displays the phase diagram obtained in the CW approximation for a homogeneous graph (regular random graph with degree $K = 5$) and for a heterogeneous graph with $P(k) \propto k^{-3.5}$. The first-order branch was determined by equating the free energy of the paramagnetic and the ferromagnetic solutions. While the lines of continuous phase transitions collapse using the rescaled variables (τ, δ), the behaviors of the discontinuous transitions remain different as they depends on the average degree $\langle k \rangle$, and not on the ratio $\langle k^2 \rangle/\langle k \rangle$. The reentrant behavior of the first-order transition line is evident in the case of heterogeneous graphs. A similar result holds for queuing models on random graphs, where the transition point that divides congested and free phases scales differently with the moments of the degree distribution for continuous and discontinuous transitions, respectively [19]. In summary, the CW approximation would suggest that in the BC model an inverse phase transition can be triggered by a different scaling of first and second order critical lines with the moments of the degree distribution. We see in the following that, although the role of degree heterogeneity is crucial to have a reentrance, this is not strictly associated to the different scaling of the first-order and second-order phase transitions.

Results in the BP Approximation. – The existence of a topology induced inverse behavior is confirmed by the more accurate Bethe-Peierls (BP) approximation [2]. On a tree-like structure emerging from a randomly chosen node i, the partition function of the system can be written as

$$Z = \sum_{s_i} e^{-\beta \Delta s_i^2} \prod_{j \in \partial_i} m_{ij}(s_i) \qquad (5)$$

where ∂_i is the set of neighbors of i and $m_{ij}(s_i)$ satisfies the recursive equation

$$m_{ij}(s_i) = \sum_{s_j} e^{\beta(s_i s_j - \Delta s_j^2)} \prod_{k \in \partial_j \setminus i} m_{jk}(s_j). \qquad (6)$$

With the parametrization $m_{ij}(s_i) = A_{ij} e^{\beta(u_{ij} s_i - v_{ij} s_i^2)}$, we can easily obtain a set of recursive equations for the *fields* u_{ij} and the *anisotropies* v_{ij}, that can be solved numerically and used to compute the local densities $p_i = \langle s_i^2 \rangle$ and local magnetization $m_i = \langle s_i \rangle$ for each node i:

$$p_i = \frac{2 \cosh(\beta \sum_j u_{ij})}{e^{\beta(\Delta + \sum_j v_{ij})} + 2 \cosh(\beta \sum_j u_{ij})}, \qquad (7)$$

$$m_i = p_i \tanh(\beta \sum_j u_{ij}).$$

In Fig.2 (left) we plot the total magnetization as a function of the temperature T in random graphs with $P(k) \propto k^{-\gamma}$ ($N = 10^4$). For all values of γ, the magnetization at $T = 0$ drops to zero for sufficiently large Δ, even if a metastable ferromagnetic phase survives at $T = 0$. The agreement between BP results (lines) and Monte Carlo simulations (points) is very good. In the right panel of Fig.2, we report the phase diagram obtained using the BP approximation for the same values of γ. The points are obtained averaging the results obtained running BP equations on given instances, while the full line is the analytic prediction of the continuous transitions and the tricritical points obtained again within the BP approximation, but solving the equations at the level of ensembles of random graphs. Indeed, for random graphs characterized only by the degree distribution $P(k)$ we can divide the nodes in classes according to their degree k and consider the cavity fields $\{u_k, v_k\}$ symmetric within each class. Once introduced the average cavity fields $\bar{u} = \sum_k P(k) u_k$ and $\bar{v} = \sum_k P(k) v_k$, one can easily check that they have to satisfy a closed set of self-consistent equations, $\bar{u} = f(\bar{u}, \bar{v})$, $\bar{v} = g(\bar{u}, \bar{v})$. The paramagnetic solution of these equations reads

$$\bar{u} = 0$$

$$\bar{v}^* = \frac{1}{\beta} \sum_k \frac{k P(k)}{\langle k \rangle} \log \frac{e^{\beta(\Delta + (k-1)\bar{v}^*)} + 2}{e^{\beta(\Delta + (k-1)\bar{v}^*)} + 2 \cosh \beta}. (8)$$

Upon expansion around this solution, the tricritical point is given by the conditions $\partial_{\bar{u}} f(0, \bar{v}^*) = 1$, $\partial_{\bar{u}}^3 f(0, \bar{v}^*) = 0$. The first equation describes the λ line of the second order critical points and gives us the value of $\Delta_c(\beta)$ as a function of the temperature while the second equation fixes the ending point of this line, β_c and its associated $\Delta_c(\beta_c)$. The previous conditions result into a set of two coupled implicit equations for β_c and Δ_c

$$\sum_k \frac{k(k-1)P(k)}{\langle k \rangle} \frac{2 \sinh \beta_c}{e^{\ell_c} + 2 \cosh \beta_c} = 1$$

$$\sum_k \frac{k(k-1)^3 P(k)}{\langle k \rangle} \frac{e^{2\ell_c} - 2e^{\ell_c} \cosh \beta_c - 8}{(e^{\ell_c} + 2 \cosh \beta_c)^3} = 0 \quad (9)$$
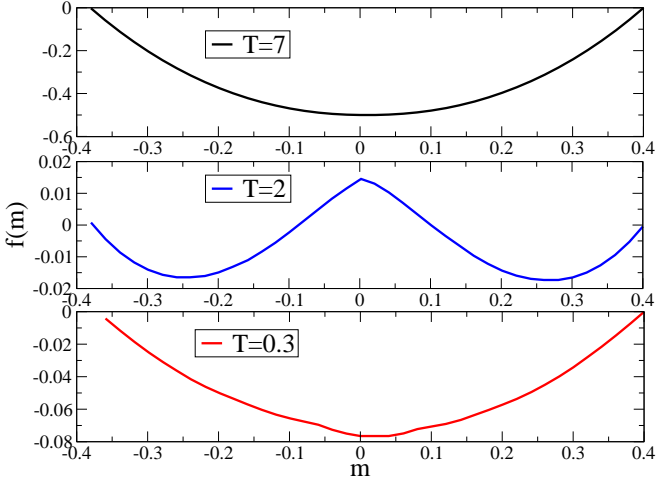
Fig. 3: The free energy computed on a single graph is shown for $\Delta = 4$ in the left panel and for $\Delta = 3$ in right panel. We use the algorithm developed in [25], by using a Legendre transformation. The scale free graph used has $N = 5000$, $k_{min} = 4$ and $\gamma = 3.5$. In both cases the free energy displays a minimum in zero for $T > T_c$ the critical temperature and, more importantly, for $T < T_m$ (the melting temperature). In between these two temperatures, $T_m < T < T_c$, it shows a ferromagnetic behavior with two minima in $\pm m$.

where $e^{\ell_c} = e^{\beta_c(\Delta_c + (k-1)\bar{v}^*)}$ These equations have been solved numerically for ensembles of power-law random graphs with $\gamma = 2.5, 3, 3.5$ (see right panel in Fig. 2).

The overall picture obtained from the CW approximation is confirmed by BP results, although the position of the tricritical point seems to move to the left of the maximum of the curve in the BP phase diagram, showing that inverse transitions can be continuous as well.

We checked that the fixed point solutions of the cavity equations have a true thermodynamic meaning by computing and plotting the Landau free energy as a function of the magnetization $f(m)$. We use the algorithm developed in [25] to reconstruct the free energy landscape by means of a Legendre transformation. The two panels reported in Fig.3 show that the free energy of a scale free graph for $\Delta = 4$ (left) and $\Delta = 3$ (right). We can see that in both cases the free energy signals the presence of a stable paramagnetic solution at high temperature, i.e. it has a minimum at $m = 0$. Then a ferromagnetic solution $m > 0$ appears at smaller temperature and finally, cooling down the system below the melting temperature T_m, it is possible to see the minimum of free energy again at the origin $m \approx 0$.

A Microscopic Mechanism for Reentrance. – By performing a low temperature analysis, we found that nodes with different degrees can have very different values of magnetization. In Fig.4(top-right) we report the magnetization curves $m(T)$ at $\Delta = 3$ for a bimodal random graph with $P(k) = 0.2\delta_{k,10} + 0.8\delta_{k,2}$ obtained by
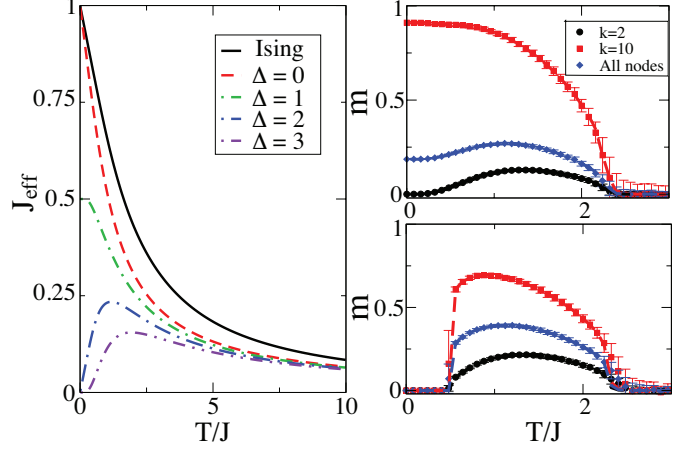

Fig. 4: Left) Effective interaction $J_{eff}(T)$ between the neighbors of a node of degree 2 as a function of the temperature T for several Δ. Right) Magnetization as a function of the temperature for $\Delta = 3$ in uncorrelated (top) and disassortative (bottom) bi- modal random graphs with $P(k) = 0.2\delta_{k,2} + 0.8\delta k, 10$. The behavior of nodes belonging to different classes of degrees is highlighted. The curves display results from both Monte Carlo simulations (points) and BP calculations (solid lines).

Monte Carlo simulations and BP calculations. The curve referring to nodes with lower degree is showing a reentrant behavior, whereas the one of high degree nodes is not. This behavior suggests that the topology-induced reentrance could be activated at low T by a complex recursive microscopic mechanism starting from the spins of lowest degree that freeze to zero for a sufficiently large chemical potential Δ. For simplicity we consider a node i of degree 2 and two neighboring nodes i_1, i_2 of degree larger than 2. At zero-temperature a chemical potential $\Delta > 2$ is sufficient to freeze $s_i = 0$ independently of the neighbors of i. Once s_i is frozen to zero, the two neighbors i_1, i_2 are not directly correlated anymore, the effective interaction is zero and the local fields acting on them do decrease. They now have to be compared with Δ to establish whether nodes i_1, i_2 are set to zero or not. Pushing forward this decimation procedure (which coincides with Δ-core percolation [20]) makes it possible to recursively determine the whole ground state of the system. We can also check how the interaction between s_{i_1} and s_{i_2} changes at finite T. If we sum over the values of the internal spin s_i, the partial partition function of the three spins becomes that of a system of two spins with an effective coupling $J_{eff} = \frac{1}{2\beta} \log \left(\frac{1 + 2e^{-\beta\Delta} \cosh(2\beta)}{1 + 2e^{-\beta\Delta}} \right)$. In the left part of Fig. 4 we show that as soon as $\Delta > 1$, the coupling between i_1 and i_2 becomes non-monotonic in T and for $\Delta > 2$ the coupling vanishes at $T = 0$ due to the freezing of $s_i = 0$. Combining the renormalization argument with the previous decimation algorithm, it is possible to check that two far-away spins remain completely uncorrelated at low T and their effective coupling increases at larger temperatures. Degree heterogeneity is the first essential

ingredient needed for an inverse transition because when all nodes have approximately the same degree, the renormalization of couplings is not effective. Another important ingredient that enhances the reentrant behavior are degree anticorrelations. In order to verify this idea, we used a Monte Carlo algorithm proposed in [22] in order to generate instances of correlated networks where high degree nodes are preferentially connected to low degree ones. An uncorrelated random graph is first generated with the configuration model. Then Monte Carlo moves are used to exchange the ends of randomly chosen link-pairs, in order to introduce positive or negative correlations among the degrees without altering the degree distribution. In the bottom-right panel of Fig.4 we show the curves $m(T)$ for the BC model in a bimodal random graph with disassortative mixing. In this case the freezing of low degree nodes at low T is sufficient to disconnect the whole graph triggering an inverse phase transition. Similarly, a low level of disassortative mixing is sufficient to enhance the reentrant behavior in scale-free graphs (not shown). Therefore, disassortative mixing favors inverse phase transitions. Unlike mean-field results, this argument is not affected by spatial fluctuations, hence we guess that a topologically induced inverse transition should be observable in dimensional lattices as well if there is a sufficient degree of local disorder and degree anti-correlation. The renormalization argument as well as the mean-field calculation can be extended to other tricritical spin models, such as the random-field Ising model (RFIM) with a bimodal distribution of fields. However, the phase diagram of this model has a complex structure of singularities even on homogeneous random graphs [24] and further investigations are needed to assess the generality of the observed phenomenon.

Conclusions. – We showed that tricritical spin systems can admit inverse phase transitions on heterogenous graphs. Mean-field arguments qualitatively suggest a different scaling of the first and second order critical point with the moments of the degree distribution for random graphs. A microscopic mechanism of coupling renormalization shows that in the presence of degree heterogeneity, the effective coupling among two nodes becomes temperature dependent. In this way, we have shown that the conditions usually described in the Flory-Huggins theory of inverse melting can have also a topological nature. The reentrant behavior is strongly enhanced (damped) by the presence of negative (positive) degree correlations.

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